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Andersen, Nick Papior; Brandbyge, Mads

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Center for Nanostructured Graphene

Technical University of Denmark

DTU

Re-implementation of TranSIESTA and *N*-terminal NEGF

Nick Papior Andersen & Mads Brandbyge

DTU Dept. of Micro- and Nanotechnology & Center for Nanostructured Graphene, DK-2800 Kgs. Lyngby, Denmark

Abstract

DFT+NEGF methods are the basis of theoretically calculating the transport properties of nanostructures. In TranSIESTA [1, 2] the NEGF implementation is currently scaling with N^3 which limits the sizes of systems, in terms of orbitals, that can be investigated. In this work we present a re-implementation of TranSIESTA which scales order-N. Using the intrinsic block-tri-diagonal form of the Hamiltonian we use the recursive Green's function method to calculate the density matrix in non-equilibrium.
We also report of TranSIESTA being extended to handle $N \geq 1$ electrodes in a generic implementation to allow the investigation of complex structures, the N-electrode setup is straight forwardly implemented and extended similarly to [3].

Re-implementation of TranSIESTA DFT-NEGF method

- Governing NEGF equations

$$\rho_{\mathrm{eq}} \propto -\frac{1}{\pi}\iint_{-\infty,\mathrm{BZ}}^{\infty} \mathrm{d}\epsilon\mathrm{d}\mathbf{k}\left[\mathbf{G}_{\mathbf{k}}(\epsilon) - \mathbf{G}_{\mathbf{k}}^{\dagger}(\epsilon)\right] n_F(\epsilon)$$

$$\rho_{\mathrm{neq}} \propto -\frac{1}{\pi}\iint_{-\infty,\mathrm{BZ}}^{\infty} \mathrm{d}\epsilon\mathrm{d}\mathbf{k}\left\{\left[\mathbf{G}_{\mathbf{k}}(\epsilon) - \mathbf{G}_{\mathbf{k}}^{\dagger}(\epsilon)\right] n_{F,\mathfrak{e}_1}(\epsilon) - \mathbf{G}_{\mathbf{k}}(\epsilon)\sum_{\mathfrak{e}\forall\mu_{\mathfrak{e}}\neq\mu_{\mathfrak{e}_1}}^{\mathfrak{E}}\Gamma_{\mathfrak{e},\mathbf{k}}(\epsilon)\left[n_{F,\mathfrak{e}}(\epsilon) - n_{F,\mathfrak{e}_1}(\epsilon)\right]\mathbf{G}_{\mathbf{k}}^{\dagger}(\epsilon)\right\}$$

- Full sparsity pattern utilisation (huge memory decrease)
- Calculating $\mathbf{G}_{\mathbf{k}}(\epsilon)$:

$$\mathbf{G}_{\mathbf{k}}^{-1}(\epsilon) = \epsilon\mathbf{S}_{\mathbf{k}} - \mathbf{H}_{\mathbf{k}} - \sum_{\mathfrak{e}}\Sigma_{\mathbf{k}}^{\mathfrak{e}}(\epsilon) = \begin{pmatrix} \boldsymbol{A}_1 & \boldsymbol{C}_2 & \mathbf{0} & & \cdots \\ \boldsymbol{B}_1 & \boldsymbol{A}_2 & \boldsymbol{C}_3 & \mathbf{0} & \cdots \\ \mathbf{0} & \boldsymbol{B}_2 & \ddots & \ddots & \\ & \mathbf{0} & \ddots & \ddots & \boldsymbol{C}_p \\ \vdots & \vdots & & \boldsymbol{B}_{p-1} & \boldsymbol{A}_p \end{pmatrix}$$

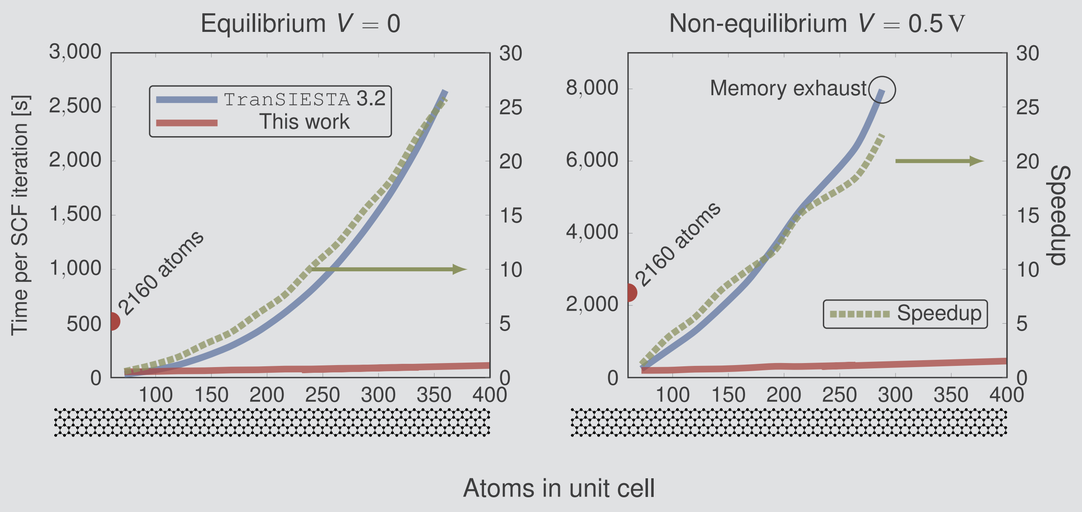
- Block-tri-diagonal (BTD) Hamiltonian is intrinsic, algorithm for inverting BTD [4, 5] (recursive Green's function method)
- Non-equilibrium contour integral correction term:

$$\Delta_{\mathbf{k}}^{\mathfrak{e}} \propto \mathbf{G}_{\mathbf{k}}(\epsilon)\Gamma_{\mathbf{k}}^{\mathfrak{e}}(\epsilon)\mathbf{G}_{\mathbf{k}}^{\dagger}(\epsilon)$$

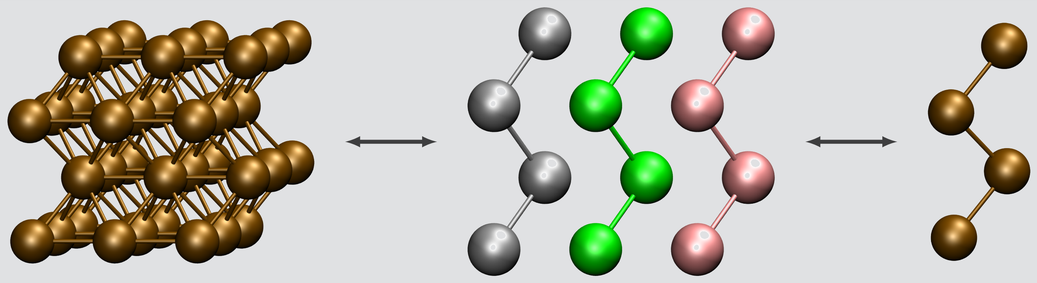
  Only part of the Greens function is needed:

$\mathbf{G}_{\mathbf{k}}(\epsilon)\Gamma_{\mathbf{k}}^{\mathfrak{e}}(\epsilon)\mathbf{G}_{\mathbf{k}}^{\dagger}(\epsilon) \rightarrow$  $\equiv$

Performance test on pristine graphene

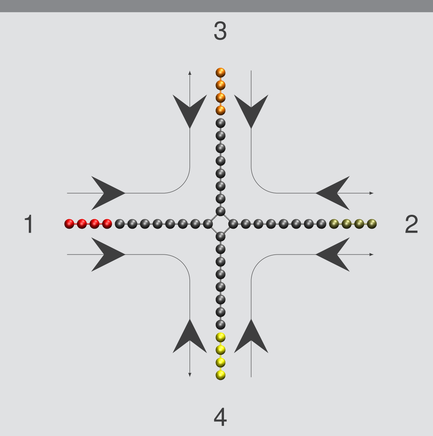


Bloch's theorem on self-energy calculations



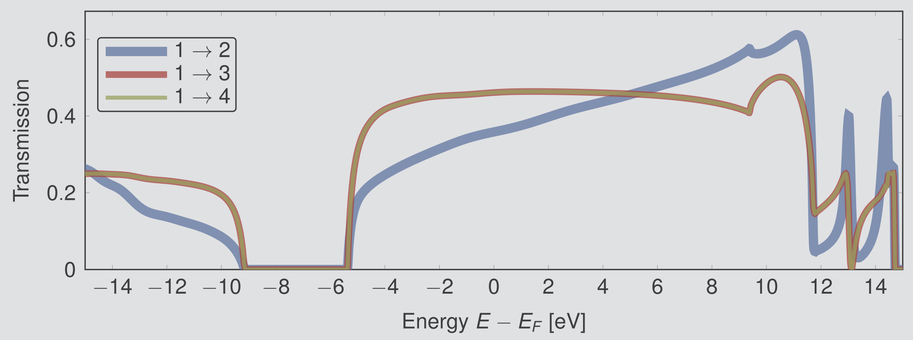
- Using the MUMPS library [6, 7], we also implement TranSIESTA in a fully sparse method allowing the user to decide amongst algorithms
- Improved contour algorithms to better approximate $\int \mathrm{d}\epsilon$ integrals
  - Gauss-Fermi quadrature re-calculated
  - Gauss-Legendre, utilise DOS position in complex plane to reduce points
  - Composite Newton-Cotes methods implemented for non-equilibrium, Simpson, Simpson 3/8, Boole
- TranSIESTA is generalised for complete N-terminal NEGF solution method
- $N = 1$ allows slab calculations using the Green's function technique which ensures a bulk slab
- $N > 2$ allows complex electrode structures
  - STM setups (3-terminal devices)
  - Molecules attached to several terminals

4-terminal carbon chain

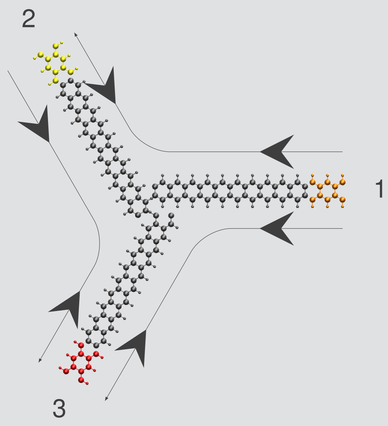


90° rotational symmetric scattering region

Transmission symmetries
- $1 \rightarrow 2 = 3 \rightarrow 4$
- $1 \rightarrow 3 = 2 \rightarrow 4$
- $1 \rightarrow 4 = 1 \rightarrow 3$

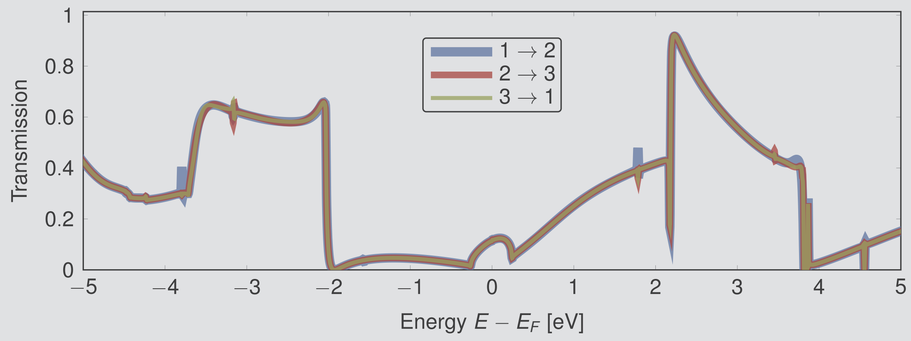


3-terminal benzene chain



120° rotational symmetric scattering region

Transmission symmetries
- $1 \rightarrow 2 = 2 \rightarrow 3$
- $1 \rightarrow 3 = 3 \rightarrow 1$



Conclusion

- Re-implemented TranSIESTA to realise bigger simulation cells
- Using recursive Green's function methods we achieve an order-N scaling for extended systems
- Implemented a fully sparse solution method which is based on the MUMPS library
- Reducing computational load by only calculating *what is needed*
- Utilising Bloch's theorem we reduce complexity of periodic electrodes by expanding self-energies
- Improved algorithms for estimating the integration in the complex plane and along the real-axis
- Generalised TranSIESTA to handle N-electrodes, taking advantage of the above mentioned computational improvements

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DTU Nanotech
Department of Micro- and Nanotechnology

nickpapior@gmail.com